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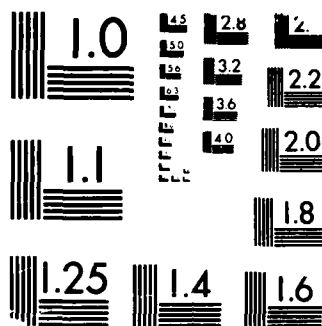
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CHAOTIC BEHAVIOUR IN QUANTUM DYNAMICS

Principal Investigator: Giulio Casati

Contractor: Centro di Cultura Scientifica "A. Volta"
Villa Olmo
22100 Como
ITALY

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First Interim Report

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CHAOTIC BEHAVIOUR IN QUANTUM DYNAMICS

Principal Investigator: Giulio Casati

First Interim Report

Since the presentation of our research proposal, we have obtained a number of results that somewhat changed the state of the art. In order to properly discuss our current work it is therefore necessary that we give a short account of these results. In Section 1 we briefly review some essential concepts; in Sect. 2 we summarize results of our work in 1987, and in the concluding Sect. 3 we describe our current lines of research.



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1. Review of Previous Results

Our research work is generally devoted to the investigation of the relevance of classical chaos to quantum mechanics, with special emphasis on quantum systems subjected to perturbations periodic in time. Keywords in this research field are

a) Classical Chaotic Diffusion: a classical nonlinear system subjected to a perturbation periodic in time may exhibit a "chaotic transition" for some critical value of the perturbation strength. Then its motion becomes extremely unstable and the system appears to diffuse in action space.

b) Quantum Localization: the quantization of a classically chaotic system, undergoing chaotic diffusion, produces a remarkable phenomenon, that this diffusion is strongly inhibited and even completely stopped by quantum interference, even in the quasi-classical case. The validity of the correspondence principle is not affected, because the motion of a quantum wave packet turns out to follow the classical diffusive pattern for a time t^* that diverges in the limit $\hbar \rightarrow 0$. After that time, the quantum packet does not spread any more, in contrast to the unlimited diffusion going on in the classical case.

This phenomenon is known as "quantum localization" since the discovery was made, that it is similar to the Anderson localization of solid state physics.

c) Anderson Localization The quantum dynamics of a particle on a discrete lattice of a given dimension d , with a time independent potential specified at each lattice site by a random variable has different predictions according to the value of α and to the degree of disorder. In general, exponentially localized eigenstates and pure energy spectrum are expected for strong enough disorder. For $d=1$, exponential localization holds for any disorder; for $d=2$, also, but the localization

lengths are now much larger than for $d=1$. For $d=3$, a transition (Anderson transition) is expected at some point, from localized to extended states.

d) Exponential Localization of Quasi Energy Eigenfunctions

A formal connection between the Anderson localization (c) and the Quantum Localization (b) was established in the following way. A system subjected to a time-periodic perturbation is completely described by its quasi-energy spectrum and eigenfunctions. For a special model system (the kicked-rotor) it turns out that finding q.e. eigenvalues and eigenfunctions in the momentum representation is formally equivalent to solving an Anderson-type problem in which the lattice sites are labelled by the unperturbed quantum numbers. Therefore, the Anderson localization corresponds to exponential localization of q.e. eigenstates in momentum space.

Although these results are related to the special kicked-rotator model, we have been contending that the same qualitative picture applies in full generality to the phenomenon of quantum limitation of classical diffusion. In particular, we have been making extensive use of a powerful heuristic estimate for the characteristic time τ^* (in the number of periods of the external periodic perturbation) after which the localization becomes effective. For a system with N freedoms that classically diffuses in the actions n_1, \dots, n_N with diffusion rates D_1, \dots, D_N , the quantum suppression of diffusion in the semiclassical regime takes place as soon as the time τ becomes so large that

$$\tau \gtrsim [D_1 D_2 \dots D_N]^{1/2} \tau^{N/2}.$$

The above estimate is in order of magnitude and in writing it we assumed $\hbar = 1$. For $N = 1$, this estimate yields the localization length l , via $l \sim [D\tau^*]^{1/2} = D$.

This means that a wave packet evolving from some given unperturbed eigenstate will eventually (after a time τ^*) settle to a maximum spread

over unperturbed levels $l \sim D$.

e) Microwave Ionization of Highly excited Hydrogen Atoms

A Hydrogen atom, initially prepared in a state very elongated along the direction of an external, linearly polarized, monochromatic electric field, provides perhaps the most important example of the above sketched situation, and it is also very close to physical application. Due to the almost one-dimensional nature of the considered orbits, a one-dimensional model can be used to study this problem. In the classical case, diffusive excitation occurs for a field strength ϵ larger than a critical value ϵ_{cr} for which an explicit estimate is known (*). This diffusion occurs in action space (i.e., in the variable n that corresponds to the principal quantum number upon quantization) and leads to fast ionization, so that ϵ_{cr} is actually a threshold for strong ionization. In the last few years we developed a theory for the corresponding quantum model, that was very well supported by the results of numerical simulation and should therefore be taken as a good theoretical description for the behaviour of real H-atoms in extended, highly-excited states, in microwave fields. The limits of validity of this description are discussed in detail in Ref. /1/.

f) Delocalization

The diffusive excitation and ionization occurring in the classical 1-d Hydrogen Atom are liable to the quantum limitation of chaotic diffusion, so that the classical threshold ϵ_{cr} is not in general a threshold for strong ionization in the quantum case. Indeed, for field strength $\epsilon > \epsilon_{cr}$ the classical diffusion can be stopped by interference unless an additional condition $\epsilon > \epsilon_q > \epsilon_{cr}$ is satisfied. ϵ_q was estimated by us /1/ and defines the threshold for quantum delocalization. Above ϵ_q , quantum

(*) At least in the case when the external frequency is larger than the unperturbed Kepler frequency.

localization is not effective and unlimited diffusion takes place in the quantum as in the classical case.

2. Survey of Recent Results

Since the classical chaotic diffusion provides a very efficient route to ionization it is interesting to investigate how the quantum delocalization border can be possibly lowered. In view of the above quoted similarity of the "dynamical" localization phenomenon for periodically perturbed quantum systems with the Anderson localization phenomenon for a random potential, one would expect that, in order to make localization less effective, the 'dynamical' counterpart of a discrete lattice of dimension higher than one should be considered (compare point (c) of the previous section).

A straightforward way to do so would seem just to consider a two-dimensional model for a highly excited hydrogen atom in a microwave field. On the other hand, the correspondence between "dynamical" and Anderson localization was derived and analyzed for the special case of the kicked rotator. Even though our extrapolation of results obtained for the rotator model to the H-atom problem was fully justified by results of numerical simulation, a closer theoretical analysis of the possible connections between the rotator and the H-atom appeared to be necessary in order that the actual relevance of localization theory for the problem of microwave ionization might be assessed.

We succeeded in doing this, by appropriately formulating the H-atom dynamics in terms of what we have called the "Kepler map" description /2/.

The idea was that the classical dynamics of the 1-d Hydrogen atom in a monochromatic electric field of strength ϵ and frequency ω , defined by the Hamiltonian

$$H = 1/2 p^2 - 1/x + \epsilon x \cos \omega t \quad (1)$$

could be efficiently, though approximately, described by a map relating the values of appropriate dynamical variables N, ϕ at subsequent passages at the aphelion. N was chosen as the unperturbed electron energy divided by ω , i. e., $N = E/\omega = -1/2n^2\omega$, n being the unperturbed action variable; instead, ϕ was defined as the field phase at perihelion. The change $\delta N = \bar{N} - N$ between the consecutive aphelion passages could be perturbatively computed as the work done by the external field along an unperturbed electronic orbit, i.e.

$$\delta N \sim -\epsilon\omega^{-1} \int_{t_1}^{t_2} \dot{x}_{\text{unp}}(t) \cos \omega t \, dt \quad (2)$$

t_1, t_2 being the times of passages at aphelion. Being interested in the case of very excited states, we can take $\dot{x}_{\text{unp}}(t) \sim \pm 2^{2/3} 3^{-1/3} |t|^{-1/3}$ which is just the unperturbed orbit of zero energy ("parabolic" orbit) and let $t_1 \rightarrow -\infty, t_2 \rightarrow +\infty$ in (2). Thus we get

$$\begin{aligned} \delta N &\sim -2^{5/3} 3^{2/3} \pi^{1/2} \epsilon \omega^{-5/3} \text{Ai}'(0) \sin \phi \\ &\approx -2.58 \epsilon \omega^{-5/3} \sin \phi \end{aligned} \quad (3)$$

$\text{Ai}'(x)$ being the derivative of the Airy function. As to the change in ϕ , at the lowest order it is given by ω times the kepler period, so that we finally get the map

$$\begin{aligned} \bar{N} &= N - K \sin \phi \\ \bar{\varphi} &= \varphi + 2\pi\omega [-2\omega\bar{N}]^{-3/2} \quad k = 2.58 \epsilon \omega^{-5/3} \end{aligned} \quad (4)$$

This map is fairly close to the standard map -i.e., to the kicked rotator- to which it can actually be reduced by linearization. This linearization procedure allows for a straightforward stability analysis, leading to the already known threshold ϵ_{cr} for the onset of chaotic motion.

The main difference of (4) from the kicked rotator is that it carries some points (N, ϕ) into the positive energy region $N > 0$, where the map itself is not defined. This corresponds to ionization.

The map (4) provides the sought for link between the H-atom problem and the rotator problem. A direct quantization of (4) can then be performed. The essential difference from the kicked rotator will be a dissipation accounting for the escape to $N > 0$. Were it not for this dissipation, the evolution of wave packets as described by (4) when the corresponding classical motion is chaotic should be localized over the unperturbed N -eigenstates, with a localization length $l \sim k^2/2$ (the classical diffusion coefficient).

Since the change $\Delta N = \Delta E/\omega$ just gives the number of absorbed photons, we would then expect an exponential localization of the wave packet in the number of absorbed photons. On the other hand, dissipation into continuum should not be effective as long as the wave packet does not significantly populate levels beyond the 1-photon threshold. Therefore, if $l \approx k^2/2$ is significantly less than $N_j = 1/2n_0^2\omega$, (the number of photons needed to reach the continuum, starting from the initial state n_0) we should expect localization.

At the same time, the condition for the breakdown of localization is $l > N_j$, which gives

$$\epsilon > \epsilon_q \sim \omega^{7/6}/(n_0\sqrt{6})$$

provided that $\omega_0 = \omega n_0^3 > 1$. If $\omega_0 < 1$, there is no localization, and diffusive ionization occurs even in the quantum case as soon as $\epsilon > \epsilon_{cr}$.

In this way, a deep-lying connection between the H-atom problem and the kicked rotator was discovered. As an immediate benefit we got a theoretical prediction about the shape of the localized distribution over the unperturbed hydrogen levels, which should be exponential in the number of absorbed photons.

The same strategy of reducing the dynamics of the H-atom in a microwave field to a mapping between subsequent passages at the aphelion proved successfull also for the study of the more complicated

model of a 2-dimensional atom, in which the electron magnetic quantum number along the direction of the field is zero. Since this number is a constant of the motion, the classical orbit would develop in a fixed plane containing the direction of the field. Unperturbed canonical variables can be chosen as n ("principal quantum number"), l (orbital momentum), with conjugated phases ϕ, ψ . The phase ψ can be chosen as the angle between the major axis of the Kepler ellipse and the direction of the field.

A map can then be derived, as was done in the 1-d case, to describe the changes of $N = -1/2n^2\omega$, $\psi = \omega t$, l, ψ between two subsequent passages at the aphelion under the given monochromatic field. This map has a complicated form, but its analysis showed that, as long as the evolution of eccentric orbits, close to parabolic ones, is considered, the evolution of N, ψ is essentially the same as described by the 1-d map (4). Instead, the evolution of the other freedom described by the (l, ψ) variables, is essentially a precession. In the chaotic regime the time scale associated with this precession is much longer than the time scale of the diffusion in energy, so that its influence on the ionization process is negligible.

In other words the classical excitation-ionization process in the 2d case is qualitatively very similar to the 1d case. In the quantum case, the main (N, θ) motion, which is classically diffusive, would be subject to localization if considered alone. Were the (l, ψ) motion negligible, one would then have a discrete q.e. spectrum. The effect of the (l, ψ) motion is a broadening of the discrete lines of this (N, θ) spectrum. A quantitative estimate of the field strength which would be necessary in order that this broadening may destroy the quasi-discrete character of the q.e. spectrum shows that this cannot happen below the 1-d delocalization border. Therefore, the conditions for intense excitation in the 2-d case are the same as in the 1-d case, and the localization picture is not affected by the addition of the 2nd freedom.

3. Current lines of research

In view of the above results, the localization phenomenon of the H-atom in a microwave field appears to be as effective in the 2-d case as it

was found to be in the 1-d one. It is not therefore connected with a very special choice of strictly 1-dimensional initial states, which greatly enhances the possibility of its experimental verification. Experimental work aimed at this purpose is now in progress /3/. According to our theory, for $\omega_0 > 1$ a significant deviation of the experimental ionization thresholds from the classically predicted ones should occur. The extent of this deviation will depend however on the details of the experimental arrangements, where ionization is identified with excitation above some fixed high-lying level \bar{n} . The theoretical border ϵ_q refers instead to excitation into continuum, and we must expect the actually observed borders to be somewhat lower due to the finite value of \bar{n} . In order to correctly interpretate forthcoming experimental data we need a theoretical prediction for the "practical" threshold which we are currently working out both theoretically and numerically.

On the other hand, the question is still open, how localization may be destroyed, in order to get strong ionization at low frequencies according to the classical predictions. A very promising way appears to be the introduction of a second perturbing frequency incommensurate with the first one. Indeed, results were already obtained by other authors, that a 2nd incommensurate frequency in the rotator case would significantly enlarge the localization lengths. This case would correspond to a 2-dimensional Anderson problem. Since, as above explained, in order to ionize a Hydrogen atom it is sufficient to get a large enough localization length, it may be the case that a second frequency enhances the ionization rate. Work on this problem is currently in progress, the results of which will hopefully presented in a forthcoming report.

References

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